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Numerical validation framework for micromechanical simulations based on 3D imaging

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Micro Abstract
A computational framework is introduced to validate simulations at the microscale. A specimen made of cast iron is imaged via synchrotron laminography during a tensile test. The region of interest is analyzed by Digital Volume Correlation (DVC) to measure kinematic fields. Finite Element simulations, which account for the studied material microstructure, are driven by Dirichlet boundary conditions extracted from DVC measurements. Gray level residuals are assessed for validation purposes.

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1 Introduction

From an industrial point of view, predicting ductile fracture, say during metal forming processes, is a top priority. This is why numerous scientific studies were conducted over the last 50 years in order to be able to predict the initiation of ductile fracture for various manufacturing conditions. Despite all these studies, there is no universal theory and predicting ductile failure is still challenging. This is due to the complexity of the thermomechanical and metallurgical mechanisms occurring during forming processes, namely, the material can be submitted to large plastic strains under multiaxial and non-proportional loading conditions, and thermal effects together with plastic strains can lead to microstructure changes. At the component scale, the prediction of ductile fracture is usually addressed using uncoupled failure criteria, coupled continuum damage mechanics approaches or damage models based on porous-plasticity theory (e.g., see Ref. [2] for a comparison of such approaches for cold metal forming applications). These approaches do not explicitly account for the material microstructure and phenomena such as the influence of elongated particles on damage anisotropy or nucleation/coalescence mechanisms are difficult to address.

The objective of this work is to study the intimate interaction between plasticity and damage mechanisms at the micrometer scale during ductile failure in the material bulk for different levels of stress triaxialities and Lode angles, and to understand the underlying physical mechanisms. To achieve this goal, three modern techniques are seamlessly coupled, namely, laminography to image in situ tested large flat samples made of ductile materials [5], global digital volume correlation (DVC) to measure 3D displacement (and strain) fields in the bulk [6], and 3D finite element (FE) simulations using the experimental information on multiple length-scales [7].

2 Numerical framework

The proposed numerical framework is exemplified for a flat specimen with central hole made of spheroidal graphite cast iron and imaged via *in-situ* synchrotron laminography at micrometer resolution during a tensile test. The region of interest in the reconstructed volume, which is close to the central hole, is analyzed by DVC to measure kinematic fields. FE simulations, which account for the morphology of the studied material microstructure, are driven by Dirichlet boundary conditions extracted from DVC measurements. Gray level residuals for DVC measurements and FE simulations are assessed for validation purposes.

The methodology proposed to obtain such local and dense comparisons between experimental analyses and numerical simulations at the microscale is based on the following steps (Figure 1):

- X-ray laminography to acquire 3D images of an *in-situ* test in a synchrotron facility [3]. By post-processing them, one may get, for instance, a first estimate of the morphology of the two-phase microstructure.

- Global DVC to measure displacement fields whose kinematic basis is made of the shape functions of 8-noded elements [6]. These displacement fields serve two purposes. First, they correspond to the kinematic data of the test. Second, they will be used as Dirichlet boundary conditions of FE simulations at the microscale.

- The FE simulations at the microscale explicitly account for the morphology of the studied two-phase material. Therefore the mesh made of 4-noded tetrahedra is adapted to the microstructure with a Level-Set procedure [9].

- FE simulations are run with an elastoplastic constitutive equation (Ludwik's law) to model the nonlinear behavior of the matrix.

- Comparisons between experimental measurements and numerical simulations are carried out for the displacement fields and more importantly the correlation residuals [1, 8].

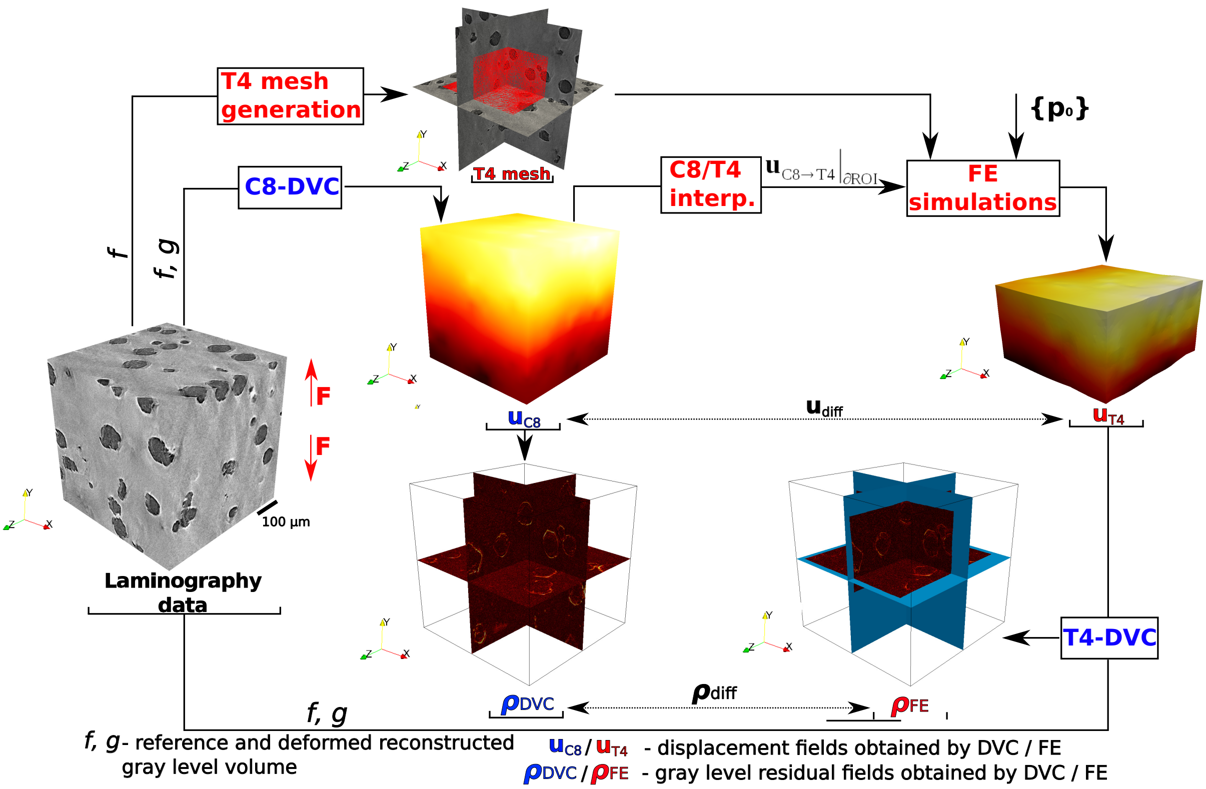

Figure 1. Schematic representation of the methods used for validating numerical simulations at the microscale (after Ref. [1])

3 Summary of findings

DVC results are validated with respect to experimental data through the correlation residuals, which are probed for all voxels belonging to the region of interest and all analyzed scans [1, 8]. Since the kinematic basis utilized herein prescribes C_0 continuity to the kinematic fields, the gray level residual fields serve as correlation quality inspector and provide a useful tool for damage detection in the zones where the continuity requirement is not met. The overall residual levels are reasonably low thereby indicating successful registrations. The areas of higher residuals correspond to the position of the debond zones that appear very early on, and increase further due to void coalescence.

Once validated, DVC measurements are used to drive FE simulations. Added to the fact that the real microstructure is discretized in the FE mesh, heterogeneous displacements prescribed by DVC require a robust mesh adaption methodology [1]. The latter is used herein and enables the simulations to be performed with significant void growth up to coalescence. While microstructures are often idealized in the literature, the present results open new possibilities for numerical modeling of heterogeneous 3D microstructures having a complex morphology and undergoing large deformations and complex topological events such as those observed in reality.

DVC and FE results are then probed by direct comparison of the full-field solutions and computation of the gray level residuals. The first method, which is a relative comparator, provides the gap between DVC and FE kinematic fields. It is shown that differences between the two methods are mainly concentrated in the bulk of the inspected region around the nodules, while boundary zones have mostly zero differences because the boundary conditions are measured via DVC. However, just observing the displacement difference between the two methods does not yield an absolute error. Conversely, the gray level residuals can be computed *independently* for both approaches. The kinematic fields are probed by computing the deformed volume corrected by the measured or simulated displacement fields. The fact that the gray level residuals remain reasonably low for the FE simulations in the void growth regime is a partial validation. However, void coalescence is not properly captured. This last result calls for more advanced constitutive models for the matrix, the nodules and their interface with the matrix. During coalescence, void nucleation at finer scales and very large strains might play a role. It is presumably associated with damage softening. The present framework will allow, in future analyses, to test this hypothesis using more sophisticated plasticity/damage models.

One of the next steps of the present work will thus deal with the constitutive law of the matrix whose parameters can be modified to get an even better agreement between the experimental data and numerical results. Similarly, the hypothesis of considering nodules as voids can also be probed and debonding can be addressed. The proposed numerical/experimental framework will still be used with sequential or integrated identification procedures [4].

To the authors' best knowledge this is the first time 3D calculations are performed on a real microstructure and by using measured boundary conditions up to large plastic strain. This approach will enable for better understanding and modeling of damage mechanisms at microscale levels. The presented numerical framework can easily be generalized for other types of materials that possess heterogeneous microstructures.

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